



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 04:12 pm GMT

PDB ID : 8Q4F  
EMDB ID : EMD-18145  
Title : Structure of arbekacin bound Escherichia coli 70S ribosome  
Authors : Majumdar, S.; Parajuli, N.P.; Ge, X.; Emmerich, A.; Sanyal, S.  
Deposited on : 2023-08-06  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

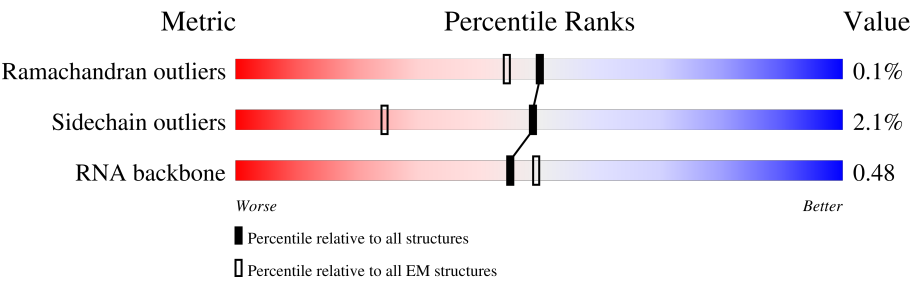
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	

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Mol	Chain	Length	Quality of chain
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	28	
28	Z	76	
29	a	2904	
30	b	120	
31	c	273	
32	d	209	
33	e	201	

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Mol	Chain	Length	Quality of chain
34	f	179	
35	g	177	
36	i	142	
37	j	123	
38	k	144	
39	l	136	
40	m	127	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	s	100	
46	t	104	
47	u	94	
48	v	85	
49	w	78	
50	x	63	
51	y	59	
52	z	57	

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 137440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1512	Total	C	N	O	P	0	0
			32450	14473	5962	10503	1512		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1197	747	228	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	127	Total	C	N	O	S	0	0
			1019	632	206	179	2		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	116	Total	C	N	O	S	0	0
			869	536	172	158	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	ASP	ASN	conflict	UNP P0A7R9

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			944	583	195	162	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 27 is a RNA chain called mRNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 28 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 29 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2732	Total	C	N	O	P	0	0
			58675	26173	10829	18941	2732		

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	208	Total	C	N	O	S	0	0
			1556	974	286	292	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	142	Total	C	N	O	S	0	0
			1123	711	209	199	4		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	134	Total	C	N	O	S	0	0
			1055	675	200	175	5		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	n	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	p	54	Total	C	N	O	0	0
			431	270	96	65		

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	t	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 47 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 48 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 49 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	62	Total	C	N	O	S	0	0
			485	300	91	93	1		

- Molecule 51 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is Arbekacin (three-letter code: 84G) (formula: C<sub>22</sub>H<sub>44</sub>N<sub>6</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total 38	C 22	N 6	O 10	0
53	a	1	Total 38	C 22	N 6	O 10	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Large ribosomal subunit protein bL33

Chain 0:  91% 7%



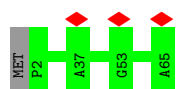
- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  100%



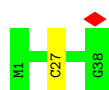
- Molecule 3: Large ribosomal subunit protein bL35

Chain 2:  5% 98%




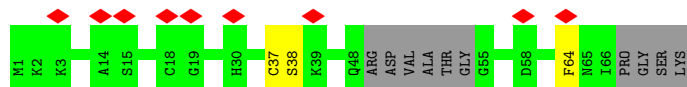
- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:  97%

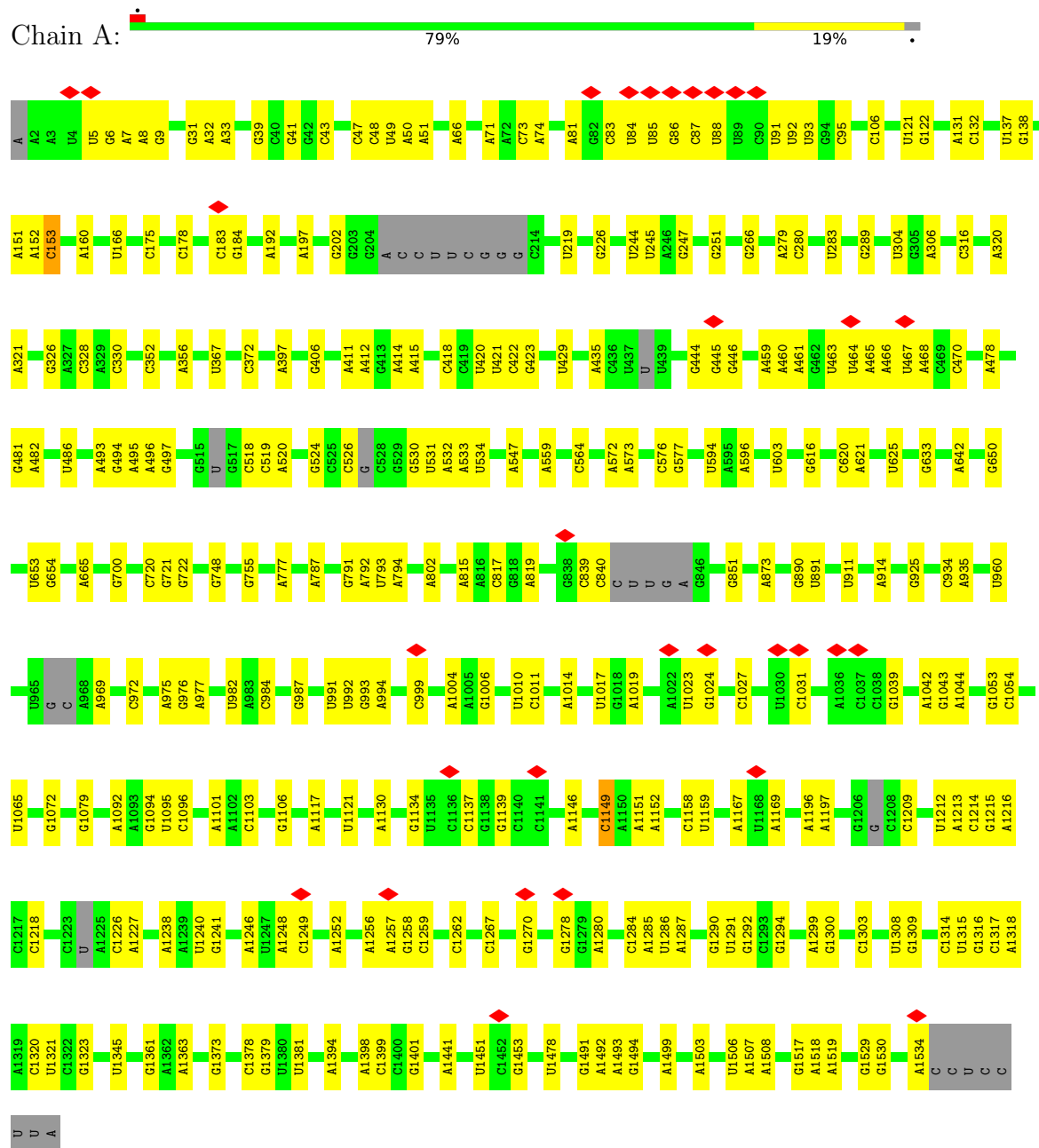


- Molecule 5: Large ribosomal subunit protein bL31A

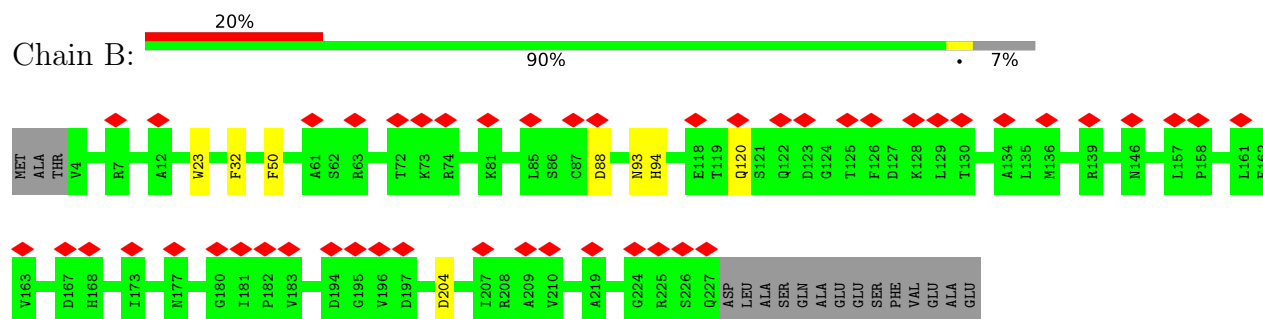
Chain 4:  13% 81% 14%




• Molecule 6: 16S rRNA

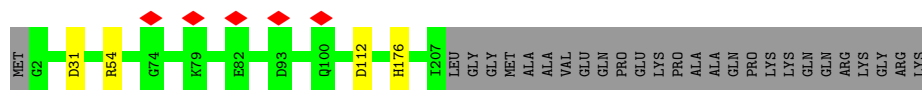


• Molecule 7: Small ribosomal subunit protein uS2



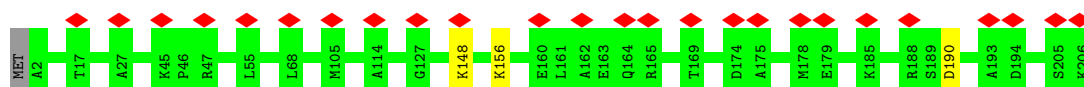
- Molecule 8: Small ribosomal subunit protein uS3

Chain C:  87% 12%

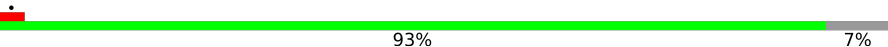


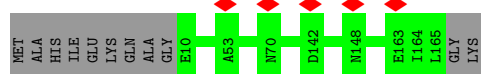
- Molecule 9: Small ribosomal subunit protein uS4

Chain D:  12% 98%




- Molecule 10: Small ribosomal subunit protein uS5

Chain E:  93% 7%




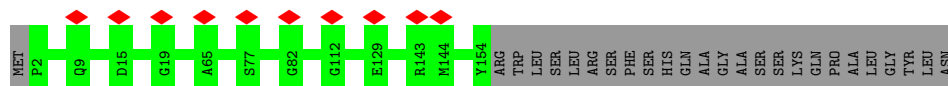
- Molecule 11: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:  76% 24%



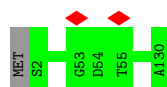
- Molecule 12: Small ribosomal subunit protein uS7

Chain G:  6% 85% 15%

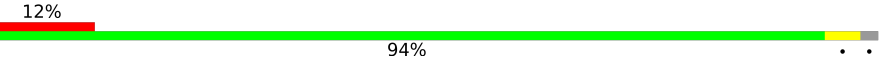


- Molecule 13: Small ribosomal subunit protein uS8

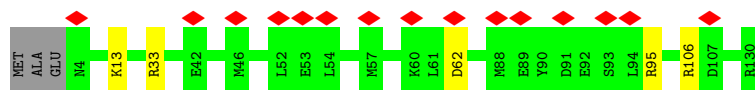
Chain H:  99%



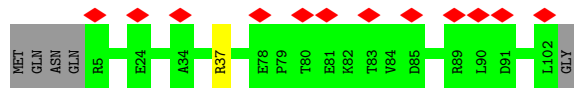
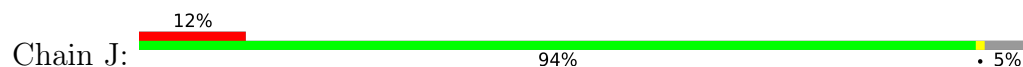
- Molecule 14: Small ribosomal subunit protein uS9

Chain I:  12% 94%

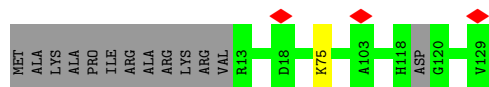
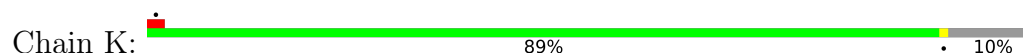




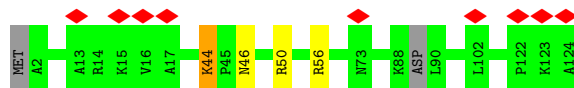
- Molecule 15: Small ribosomal subunit protein uS10



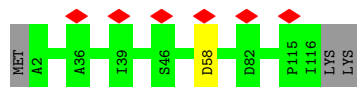
- Molecule 16: Small ribosomal subunit protein uS11



- Molecule 17: Small ribosomal subunit protein uS12



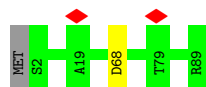
- Molecule 18: Small ribosomal subunit protein uS13



- Molecule 19: Small ribosomal subunit protein uS14



- Molecule 20: Small ribosomal subunit protein uS15



- Molecule 21: Small ribosomal subunit protein bS16

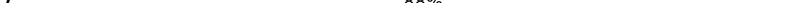
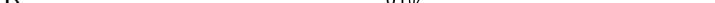
- Chain Q:  88% 6% 6%

Diagram illustrating the structure of the 14-residue peptide sequence: MET-THR-ASP-K4-D15-F28-V29-K30-H31-P32-D48-A82-VAL-LEU. The residues are color-coded: MET, THR, and VAL are grey; ASP, K4, D15, F28, V29, K30, H31, P32, and D48 are yellow; and K4, D15, V29, and A82 are green. Red diamonds are placed above the K4, D15, and V29 residues.

- Chain R:  81% 7% 12%

Sequence logo for the 1000bp upstream region of the E16 gene. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows amino acid positions from MET to GLN. A red diamond marks the E16 start site. A green bar highlights the T71 start site. A grey bar highlights the T74 start site.

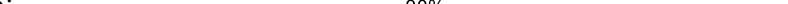
- Chain S: 

Diagram illustrating the protein structure of the 12S oxygen binding domain of hemoglobin. The structure is shown as a ribbon diagram with various residues highlighted in green and yellow. Red diamonds indicate specific residues: MET, P2, A22, S25, G26, D27, K28, K29, F41, E65, A84, and A85. The residues are arranged in a sequence from left to right: MET, P2, A22, S25, G26, D27, K28, K29, F41, E65, A84, A85, ASP, LYS, LYS, ALA, LYS, LYS, LYS.

- Chain T:  6% 99%

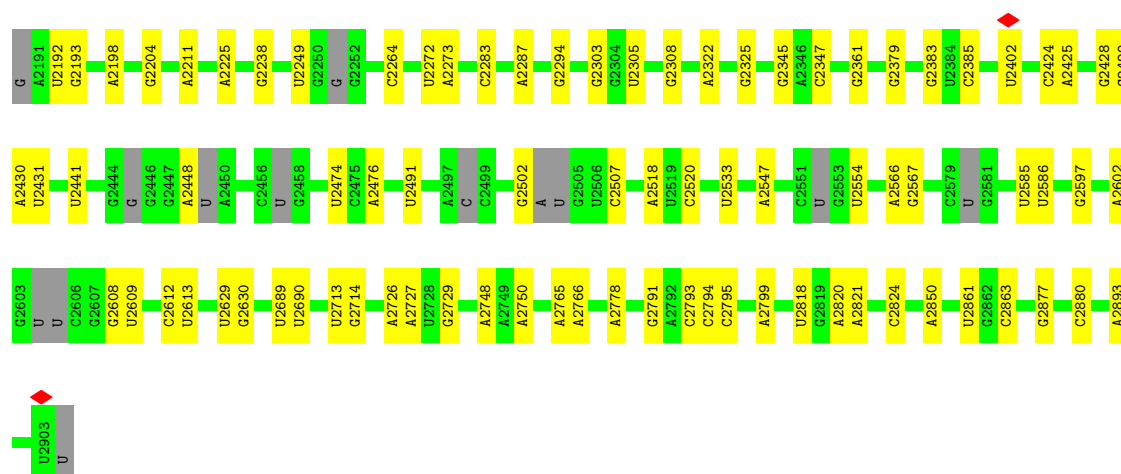
The diagram illustrates the domain structure of the A22 protein. It consists of several domains: a MET domain (grey), an A2 domain (green), an A22 domain (green), an A41 domain (green), an N84 domain (green), an K85 domain (green), an L86 domain (green), and an A87 domain (green). Red diamonds indicate the positions of mutations: A22, A41, N84, K85, and A87.

- Chain U:  13% 99%

- Chain X:  11% 89%

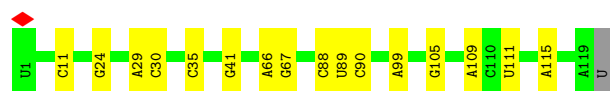
G U A U A A G G A G G U U A A A A A16 U17 G18 G U A U A A A C U A





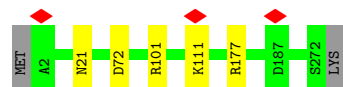
• Molecule 30: 5S rRNA

Chain b: 86% 13%



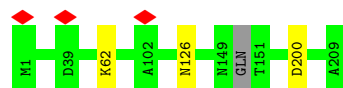
• Molecule 31: Large ribosomal subunit protein uL2

Chain c: 97%



• Molecule 32: 50S ribosomal protein L3

Chain d: 98%



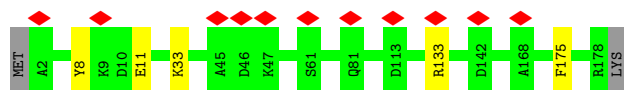
• Molecule 33: Large ribosomal subunit protein uL4

Chain e: 98%

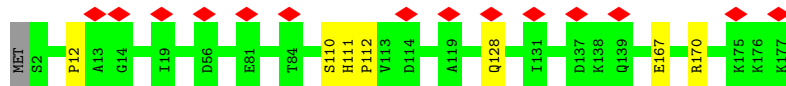


• Molecule 34: Large ribosomal subunit protein uL5

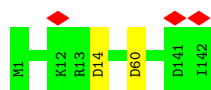
Chain f: 6% 96%



- Molecule 35: Large ribosomal subunit protein uL6



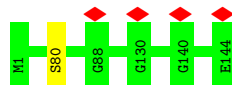
- Molecule 36: Large ribosomal subunit protein uL13



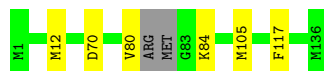
- Molecule 37: Large ribosomal subunit protein uL14



- Molecule 38: Large ribosomal subunit protein uL15



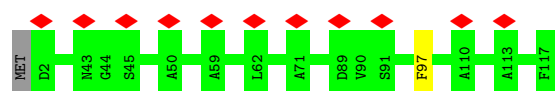
- Molecule 39: 50S ribosomal protein L16



- Molecule 40: Large ribosomal subunit protein bL17



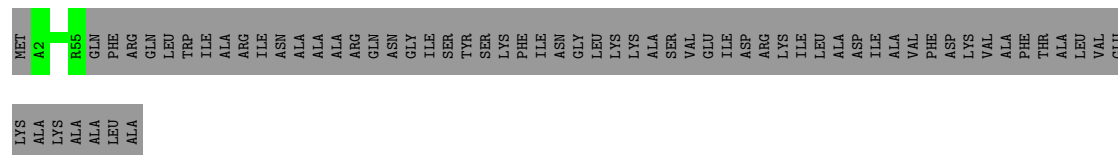
- Molecule 41: Large ribosomal subunit protein uL18



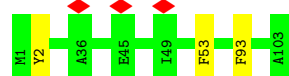
- Molecule 42: Large ribosomal subunit protein bL19



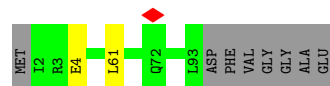
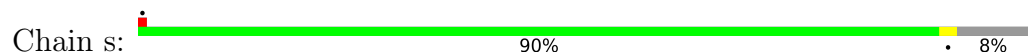
- Molecule 43: Large ribosomal subunit protein bL20



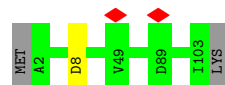
- Molecule 44: Large ribosomal subunit protein bL21



- Molecule 45: Large ribosomal subunit protein uL23



- Molecule 46: Large ribosomal subunit protein uL24

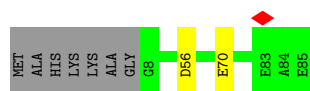
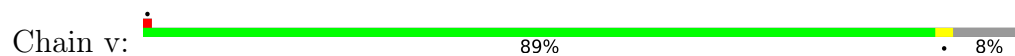


- Molecule 47: Large ribosomal subunit protein bL25

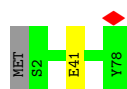




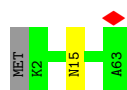
- Molecule 48: Large ribosomal subunit protein bL27



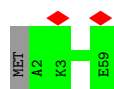
- Molecule 49: Large ribosomal subunit protein bL28



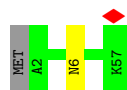
- Molecule 50: Large ribosomal subunit protein uL29



- Molecule 51: Large ribosomal subunit protein uL30



- Molecule 52: Large ribosomal subunit protein bL32



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.37	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.237	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	425.64786, 425.64786, 425.64786	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512957, 0.8512957, 0.8512957	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 84G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.53	1/424 (0.2%)	0.85	2/565 (0.4%)
2	1	0.29	0/380	0.68	0/498
3	2	0.28	0/513	0.57	0/676
4	3	0.30	0/303	0.62	0/397
5	4	0.31	0/488	0.55	0/649
6	A	0.39	0/36330	0.80	5/56657 (0.0%)
7	B	0.28	0/1784	0.53	0/2403
8	C	0.29	0/1651	0.56	0/2225
9	D	0.28	0/1665	0.55	0/2227
10	E	0.30	0/1165	0.55	0/1568
11	F	0.29	0/858	0.58	0/1160
12	G	0.28	0/1213	0.55	0/1628
13	H	0.30	0/989	0.55	0/1326
14	I	0.30	0/1031	0.63	0/1372
15	J	0.29	0/796	0.60	0/1077
16	K	0.30	0/884	0.58	0/1191
17	L	0.32	0/957	0.63	0/1282
18	M	0.28	0/900	0.61	0/1204
19	N	0.27	0/817	0.57	0/1088
20	O	0.30	0/722	0.60	0/964
21	P	0.29	0/653	0.60	0/877
22	Q	1.21	3/650 (0.5%)	1.21	6/871 (0.7%)
23	R	0.28	0/553	0.57	0/742
24	S	0.29	0/685	0.53	0/922
25	T	0.30	0/676	0.53	0/895
26	U	0.30	0/597	0.62	0/792
27	X	0.35	0/72	0.76	0/110
28	Z	0.35	0/1813	0.80	0/2825
29	a	0.43	0/65703	0.78	1/102459 (0.0%)
30	b	0.36	0/2850	0.79	0/4444
31	c	0.31	0/2121	0.59	0/2852
32	d	0.31	0/1576	0.57	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	e	0.30	0/1571	0.52	0/2113
34	f	0.29	0/1434	0.55	0/1926
35	g	0.47	2/1343 (0.1%)	0.82	7/1816 (0.4%)
36	i	0.35	0/1146	0.58	0/1544
37	j	0.32	0/955	0.66	1/1279 (0.1%)
38	k	0.31	0/1062	0.59	0/1413
39	l	0.38	1/1073 (0.1%)	0.59	0/1433
40	m	0.77	1/958 (0.1%)	1.13	5/1281 (0.4%)
41	n	0.29	0/902	0.57	0/1209
42	o	0.31	0/929	0.60	0/1242
43	p	0.32	0/436	0.65	0/578
44	q	0.34	0/829	0.59	0/1107
45	s	0.31	0/736	0.53	0/984
46	t	0.29	0/787	0.51	0/1051
47	u	0.29	0/766	0.53	0/1025
48	v	0.31	0/593	0.57	0/785
49	w	0.43	1/635 (0.2%)	0.60	0/848
50	x	0.29	0/486	0.50	0/648
51	y	0.28	0/453	0.56	0/605
52	z	0.27	0/450	0.60	0/599
All	All	0.40	9/149363 (0.0%)	0.75	27/223551 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	32	PRO	CB-CG	22.04	2.60	1.50
40	m	50	PRO	CG-CD	-20.84	0.81	1.50
22	Q	32	PRO	CG-CD	-18.74	0.88	1.50
35	g	112	PRO	CG-CD	-9.16	1.20	1.50
1	0	41	PRO	CG-CD	-7.42	1.26	1.50

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Q	32	PRO	CB-CG-CD	-24.25	11.94	106.50
40	m	50	PRO	N-CD-CG	-19.47	73.99	103.20
40	m	50	PRO	CB-CG-CD	18.82	179.90	106.50
35	g	112	PRO	CA-N-CD	-15.34	90.03	111.50
40	m	50	PRO	CA-CB-CG	-15.17	75.18	104.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
2	1	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
3	2	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
5	4	56/70 (80%)	48 (86%)	8 (14%)	0	100	100
7	B	222/241 (92%)	197 (89%)	25 (11%)	0	100	100
8	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
9	D	203/206 (98%)	187 (92%)	16 (8%)	0	100	100
10	E	154/167 (92%)	140 (91%)	14 (9%)	0	100	100
11	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
12	G	151/179 (84%)	141 (93%)	10 (7%)	0	100	100
13	H	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
14	I	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	16	48
15	J	96/103 (93%)	88 (92%)	8 (8%)	0	100	100
16	K	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
17	L	118/124 (95%)	104 (88%)	13 (11%)	1 (1%)	16	48
18	M	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
19	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
20	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
21	P	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
22	Q	77/84 (92%)	65 (84%)	12 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	R	64/75 (85%)	57 (89%)	7 (11%)	0	100	100
24	S	82/92 (89%)	76 (93%)	6 (7%)	0	100	100
25	T	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
26	U	68/71 (96%)	68 (100%)	0	0	100	100
31	c	269/273 (98%)	249 (93%)	20 (7%)	0	100	100
32	d	204/209 (98%)	191 (94%)	13 (6%)	0	100	100
33	e	199/201 (99%)	174 (87%)	25 (13%)	0	100	100
34	f	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
35	g	174/177 (98%)	153 (88%)	20 (12%)	1 (1%)	22	53
36	i	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
37	j	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
38	k	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
39	l	130/136 (96%)	124 (95%)	5 (4%)	1 (1%)	16	48
40	m	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
41	n	114/117 (97%)	99 (87%)	15 (13%)	0	100	100
42	o	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
43	p	52/118 (44%)	37 (71%)	15 (29%)	0	100	100
44	q	101/103 (98%)	90 (89%)	11 (11%)	0	100	100
45	s	90/100 (90%)	81 (90%)	9 (10%)	0	100	100
46	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
47	u	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	v	76/85 (89%)	70 (92%)	6 (8%)	0	100	100
49	w	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
50	x	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
51	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
52	z	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
All	All	5263/5654 (93%)	4828 (92%)	431 (8%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	g	128	GLN
39	l	84	LYS

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Mol	Chain	Res	Type
14	I	13	LYS
17	L	44	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	65
5	4	55/62 (89%)	52 (94%)	3 (6%)	18	47
7	B	186/199 (94%)	178 (96%)	8 (4%)	25	55
8	C	170/190 (90%)	166 (98%)	4 (2%)	44	70
9	D	172/173 (99%)	169 (98%)	3 (2%)	56	78
10	E	119/126 (94%)	119 (100%)	0	100	100
11	F	90/116 (78%)	89 (99%)	1 (1%)	70	84
12	G	125/147 (85%)	125 (100%)	0	100	100
13	H	104/105 (99%)	104 (100%)	0	100	100
14	I	104/107 (97%)	100 (96%)	4 (4%)	28	59
15	J	86/90 (96%)	85 (99%)	1 (1%)	67	83
16	K	89/99 (90%)	88 (99%)	1 (1%)	70	84
17	L	101/104 (97%)	97 (96%)	4 (4%)	27	58
18	M	93/96 (97%)	92 (99%)	1 (1%)	70	84
19	N	83/84 (99%)	81 (98%)	2 (2%)	44	70
20	O	76/77 (99%)	75 (99%)	1 (1%)	65	82
21	P	65/65 (100%)	62 (95%)	3 (5%)	23	52
22	Q	73/78 (94%)	70 (96%)	3 (4%)	26	57
23	R	57/65 (88%)	52 (91%)	5 (9%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	S	72/79 (91%)	71 (99%)	1 (1%)	62	81
25	T	65/66 (98%)	65 (100%)	0	100	100
26	U	60/61 (98%)	60 (100%)	0	100	100
31	c	216/218 (99%)	211 (98%)	5 (2%)	45	70
32	d	163/164 (99%)	160 (98%)	3 (2%)	54	76
33	e	165/165 (100%)	160 (97%)	5 (3%)	36	64
34	f	148/150 (99%)	143 (97%)	5 (3%)	32	62
35	g	137/138 (99%)	134 (98%)	3 (2%)	47	71
36	i	115/116 (99%)	113 (98%)	2 (2%)	56	78
37	j	104/104 (100%)	103 (99%)	1 (1%)	73	86
38	k	103/103 (100%)	102 (99%)	1 (1%)	73	86
39	l	107/109 (98%)	103 (96%)	4 (4%)	29	59
40	m	98/103 (95%)	96 (98%)	2 (2%)	50	74
41	n	86/87 (99%)	85 (99%)	1 (1%)	67	83
42	o	99/100 (99%)	95 (96%)	4 (4%)	27	58
43	p	37/90 (41%)	37 (100%)	0	100	100
44	q	84/84 (100%)	81 (96%)	3 (4%)	30	60
45	s	79/84 (94%)	77 (98%)	2 (2%)	42	69
46	t	83/85 (98%)	82 (99%)	1 (1%)	67	83
47	u	78/78 (100%)	77 (99%)	1 (1%)	65	82
48	v	58/63 (92%)	56 (97%)	2 (3%)	32	62
49	w	67/68 (98%)	67 (100%)	0	100	100
50	x	51/55 (93%)	50 (98%)	1 (2%)	50	74
51	y	48/49 (98%)	48 (100%)	0	100	100
52	z	47/48 (98%)	46 (98%)	1 (2%)	48	72
All	All	4387/4623 (95%)	4294 (98%)	93 (2%)	49	72

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	e	141	MET
39	l	12	MET
34	f	8	TYR

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Mol	Chain	Res	Type
35	g	167	GLU
40	m	58	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
39	l	13	HIS
41	n	116	GLN
47	u	88	HIS
15	J	56	HIS
17	L	46	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2/28 (7%)	0	0
28	Z	75/76 (98%)	10 (13%)	0
29	a	2711/2904 (93%)	356 (13%)	0
30	b	118/120 (98%)	16 (13%)	0
6	A	1503/1542 (97%)	289 (19%)	9 (0%)
All	All	4409/4670 (94%)	671 (15%)	9 (0%)

5 of 671 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	5	U
6	A	6	G
6	A	7	A
6	A	8	A
6	A	9	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1299	A
6	A	1518	A
6	A	326	G
6	A	445	G
6	A	466	A

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
53	84G	A	1601	-	39,40,40	1.90	8 (20%)	47,57,57	1.27	6 (12%)
53	84G	a	3001	-	39,40,40	1.82	7 (17%)	47,57,57	1.08	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	84G	A	1601	-	-	10/23/76/76	2/3/3/3
53	84G	a	3001	-	-	7/23/76/76	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	1601	84G	C3-N1	6.92	1.49	1.34
53	a	3001	84G	C3-N1	6.21	1.47	1.34
53	A	1601	84G	C21-C20	-4.56	1.47	1.53
53	a	3001	84G	C21-C20	-4.54	1.47	1.53
53	a	3001	84G	C19-C20	-3.60	1.49	1.53



The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	1601	84G	C4-N1-C3	-3.00	117.78	123.07
53	A	1601	84G	O6-C17-C19	2.78	114.75	109.69
53	A	1601	84G	C8-O2-C7	-2.71	111.26	117.96
53	A	1601	84G	C16-O5-C15	-2.44	111.92	117.96
53	a	3001	84G	C7-C14-C15	2.37	113.89	108.96

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

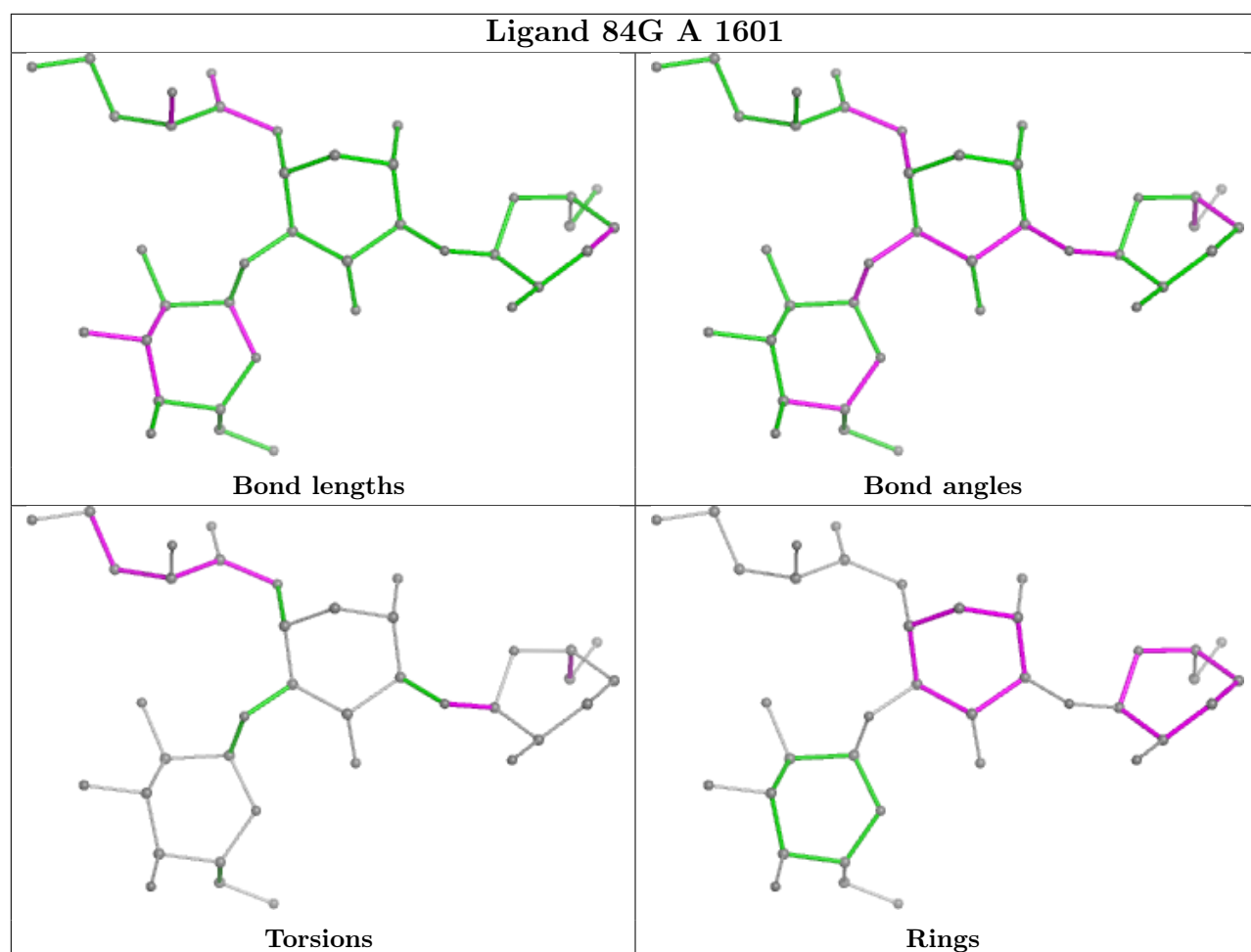
Mol	Chain	Res	Type	Atoms
53	A	1601	84G	C-C1-C2-O
53	A	1601	84G	O-C2-C3-N1
53	A	1601	84G	C2-C3-N1-C4
53	A	1601	84G	N3-C10-C9-O3
53	A	1601	84G	N3-C10-C9-C11

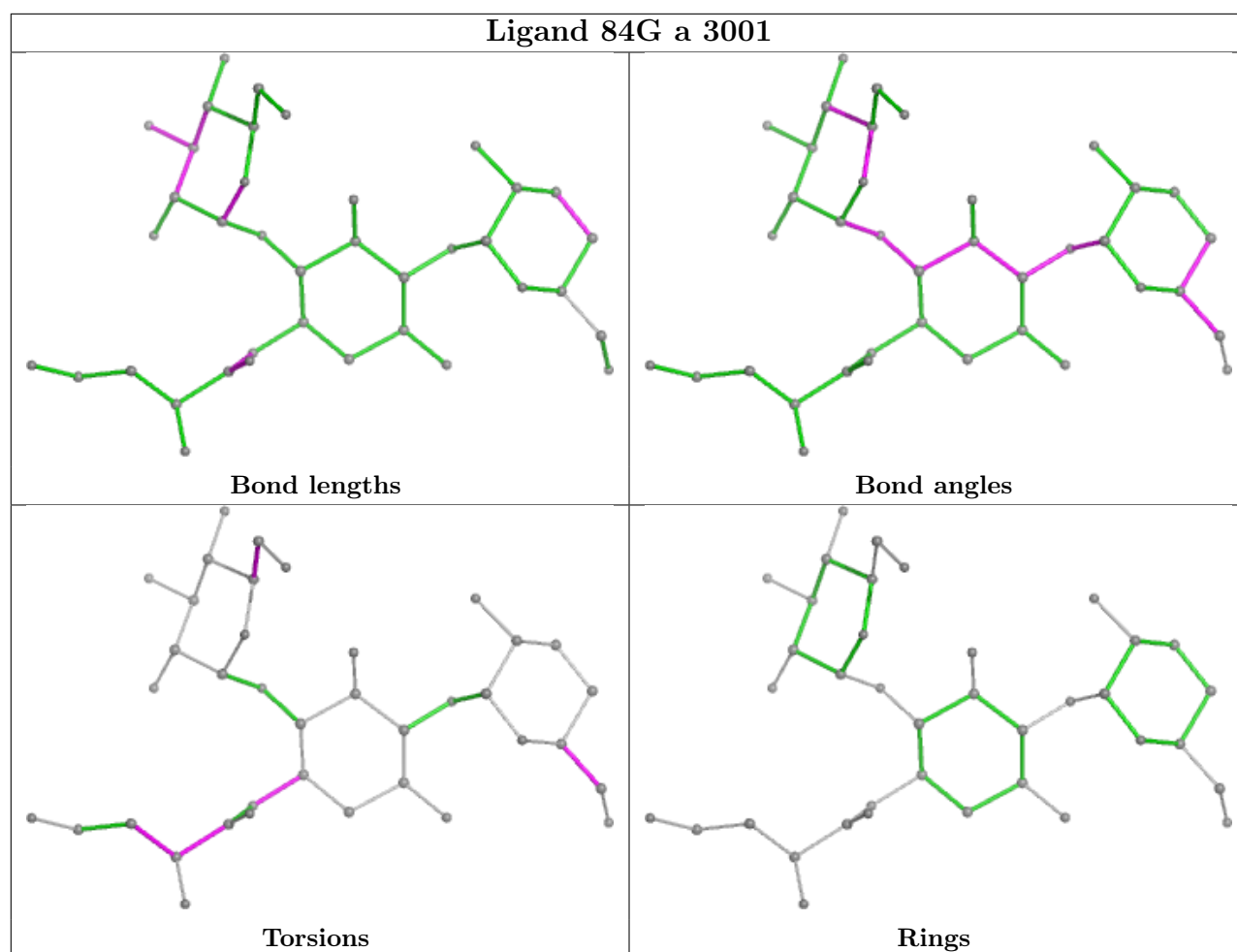
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	A	1601	84G	C14-C15-C4-C5-C6-C7
53	A	1601	84G	C11-C12-C13-C8-C9-O3

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

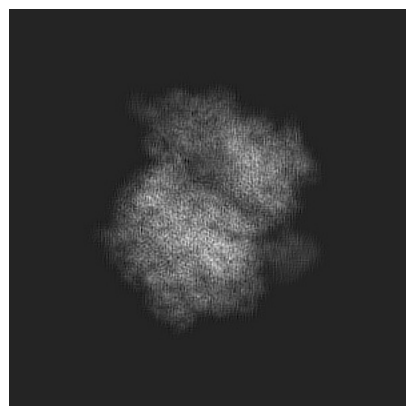
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18145. These allow visual inspection of the internal detail of the map and identification of artifacts.

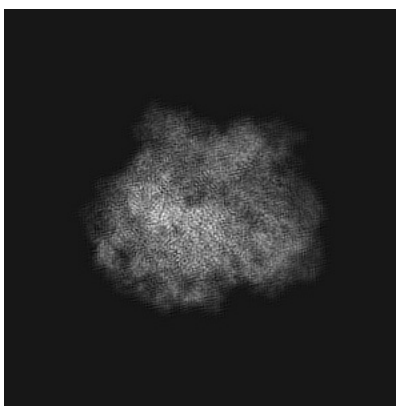
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

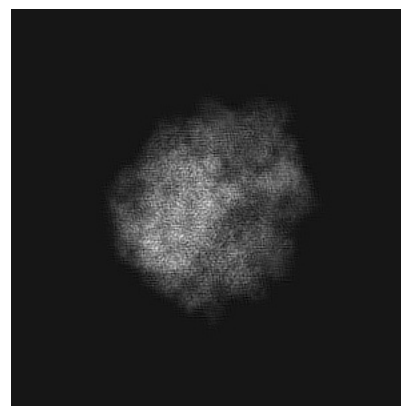
#### 6.1.1 Primary map



X

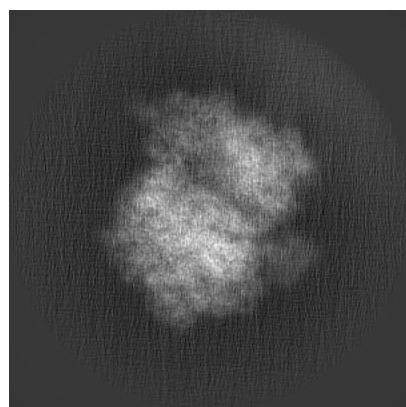


Y

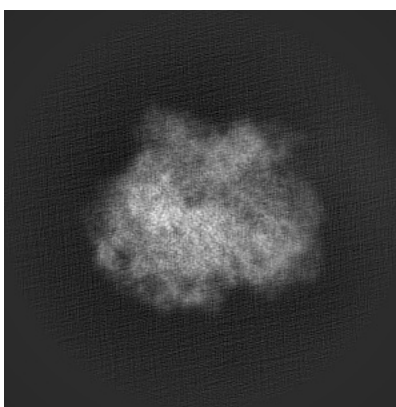


Z

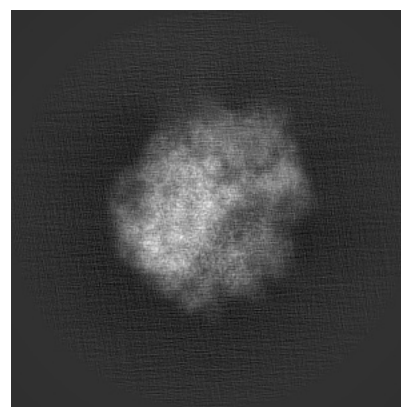
#### 6.1.2 Raw map



X



Y

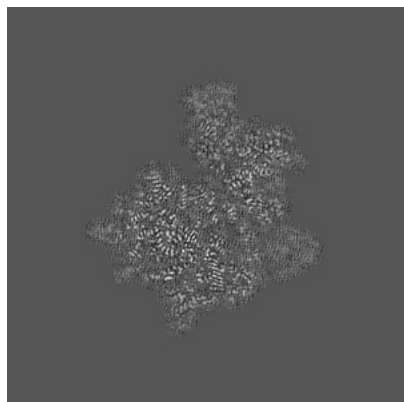


Z

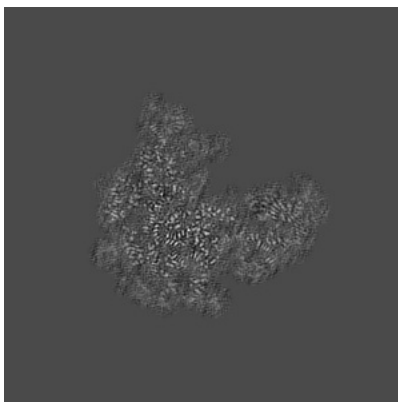
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

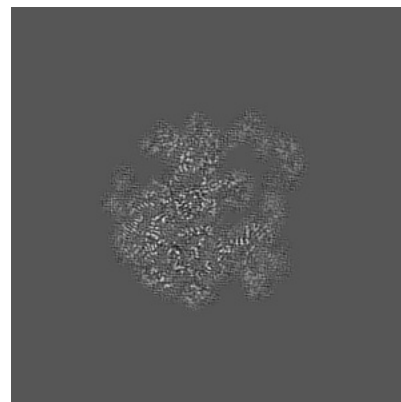
### 6.2.1 Primary map



X Index: 250

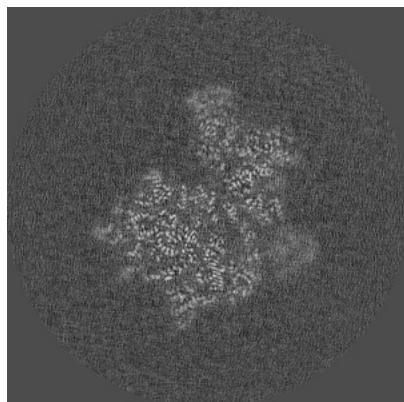


Y Index: 250

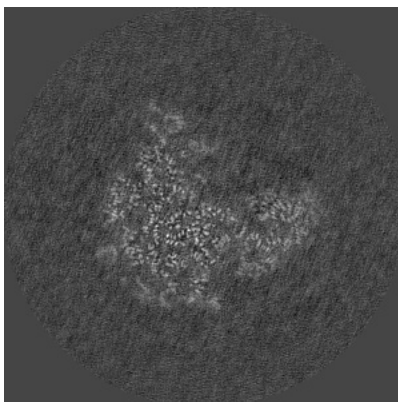


Z Index: 250

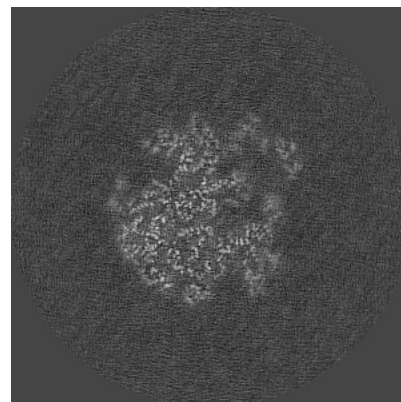
### 6.2.2 Raw map



X Index: 250



Y Index: 250

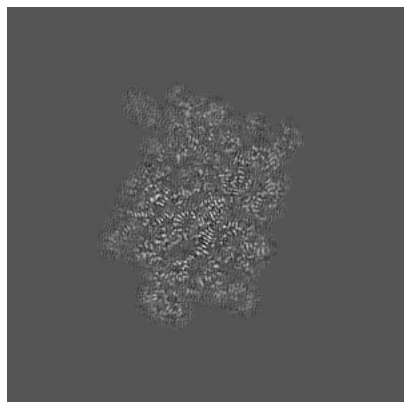


Z Index: 250

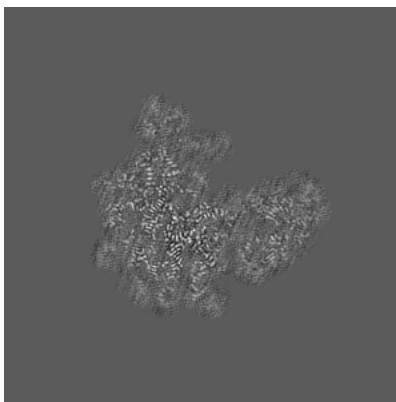
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

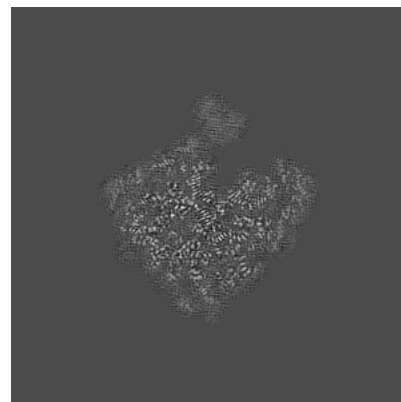
### 6.3.1 Primary map



X Index: 212

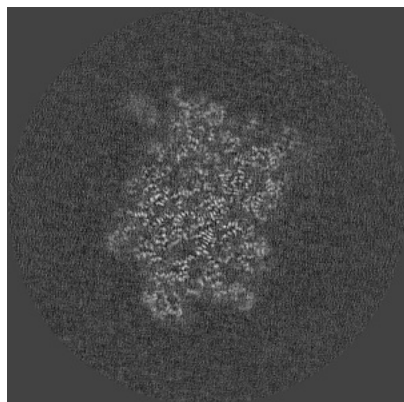


Y Index: 254

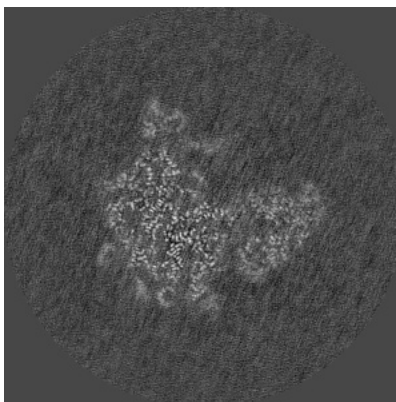


Z Index: 205

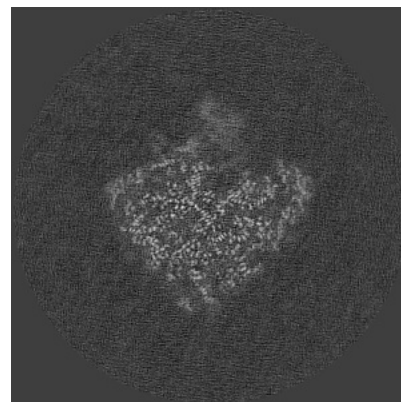
### 6.3.2 Raw map



X Index: 212



Y Index: 254



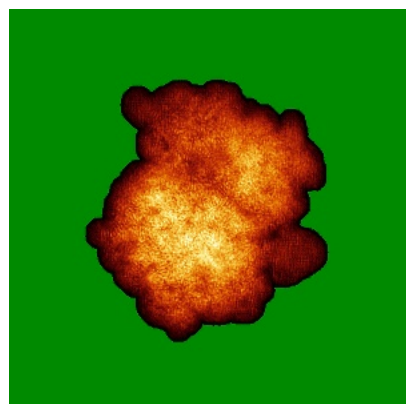
Z Index: 205

The images above show the largest variance slices of the map in three orthogonal directions.

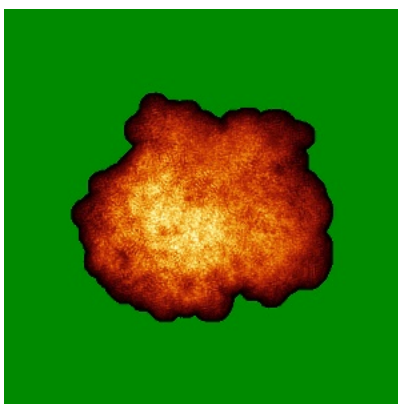


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

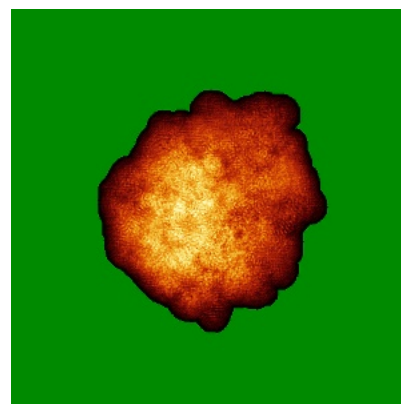
### 6.4.1 Primary map



X

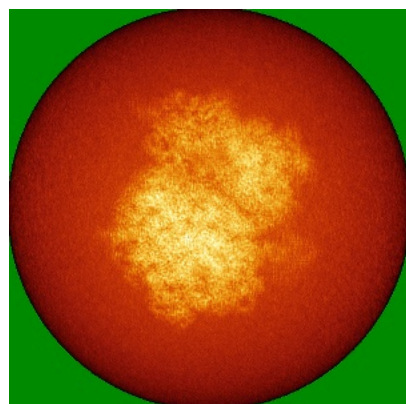


Y

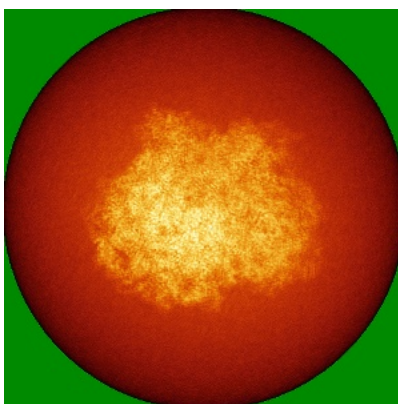


Z

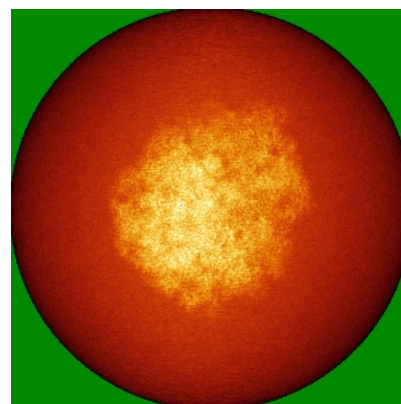
### 6.4.2 Raw map



X



Y

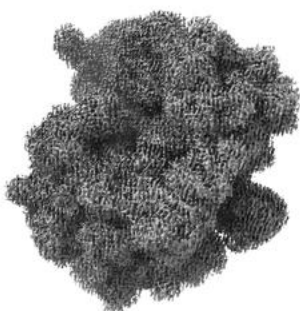


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



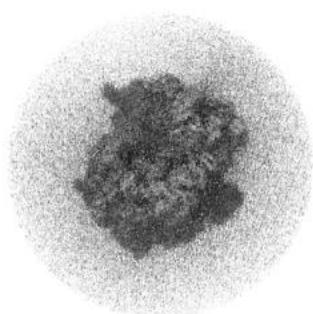
Y



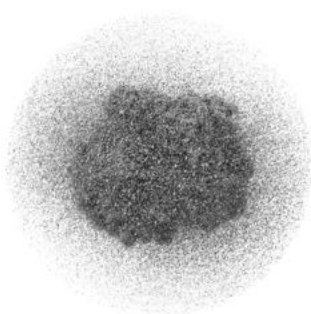
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

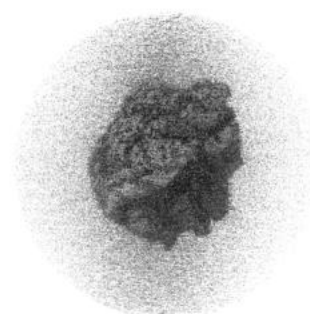
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

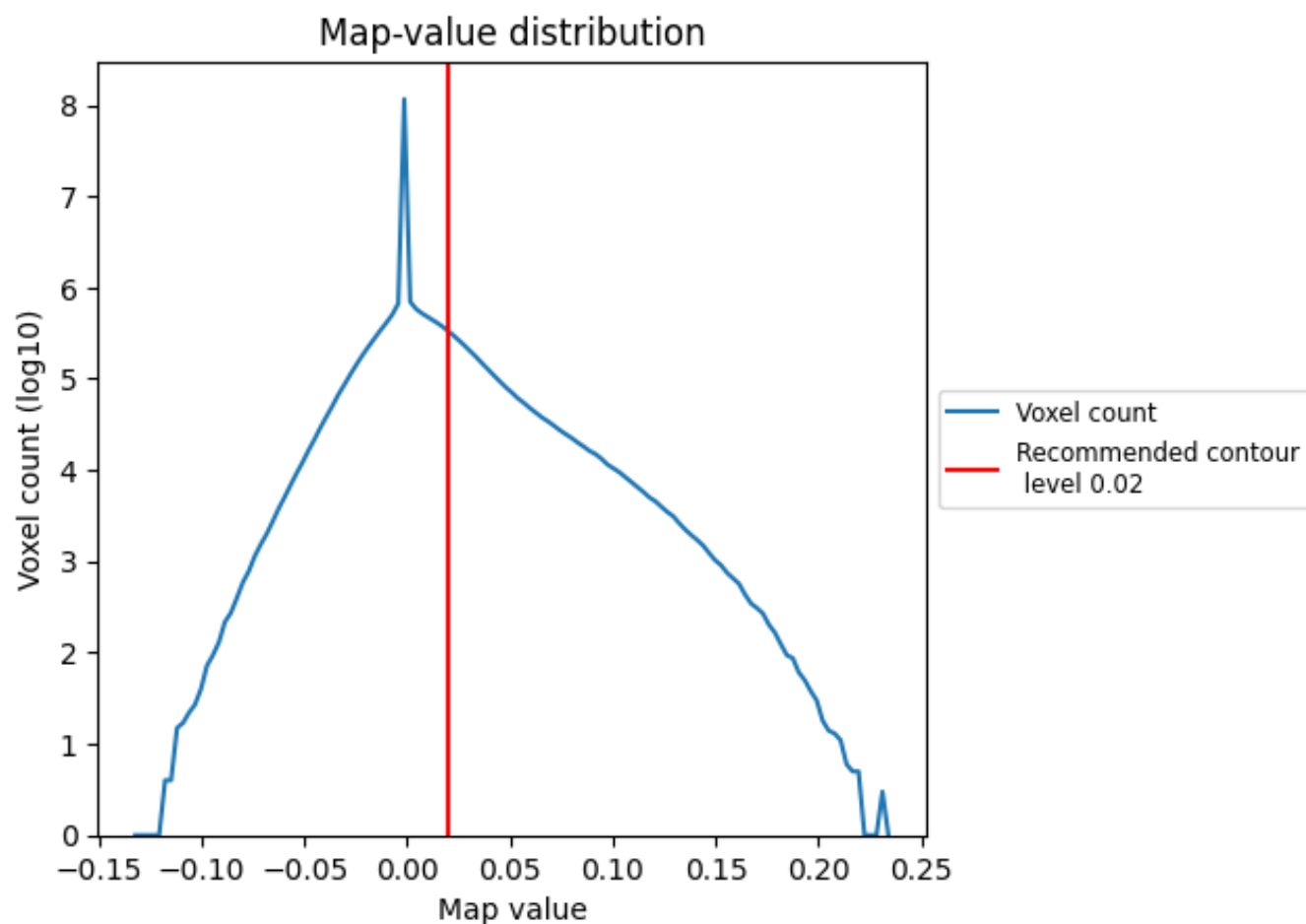
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

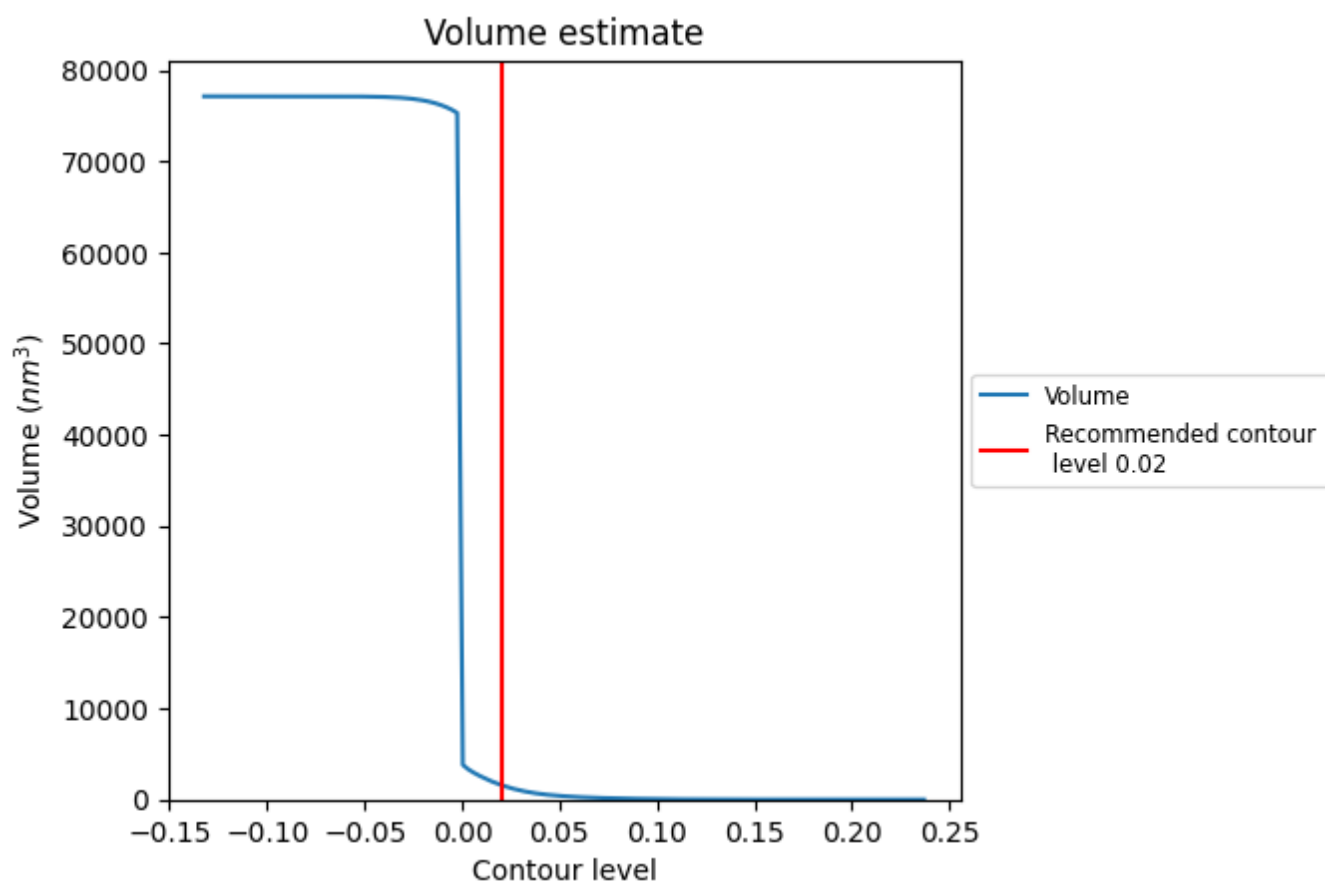
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

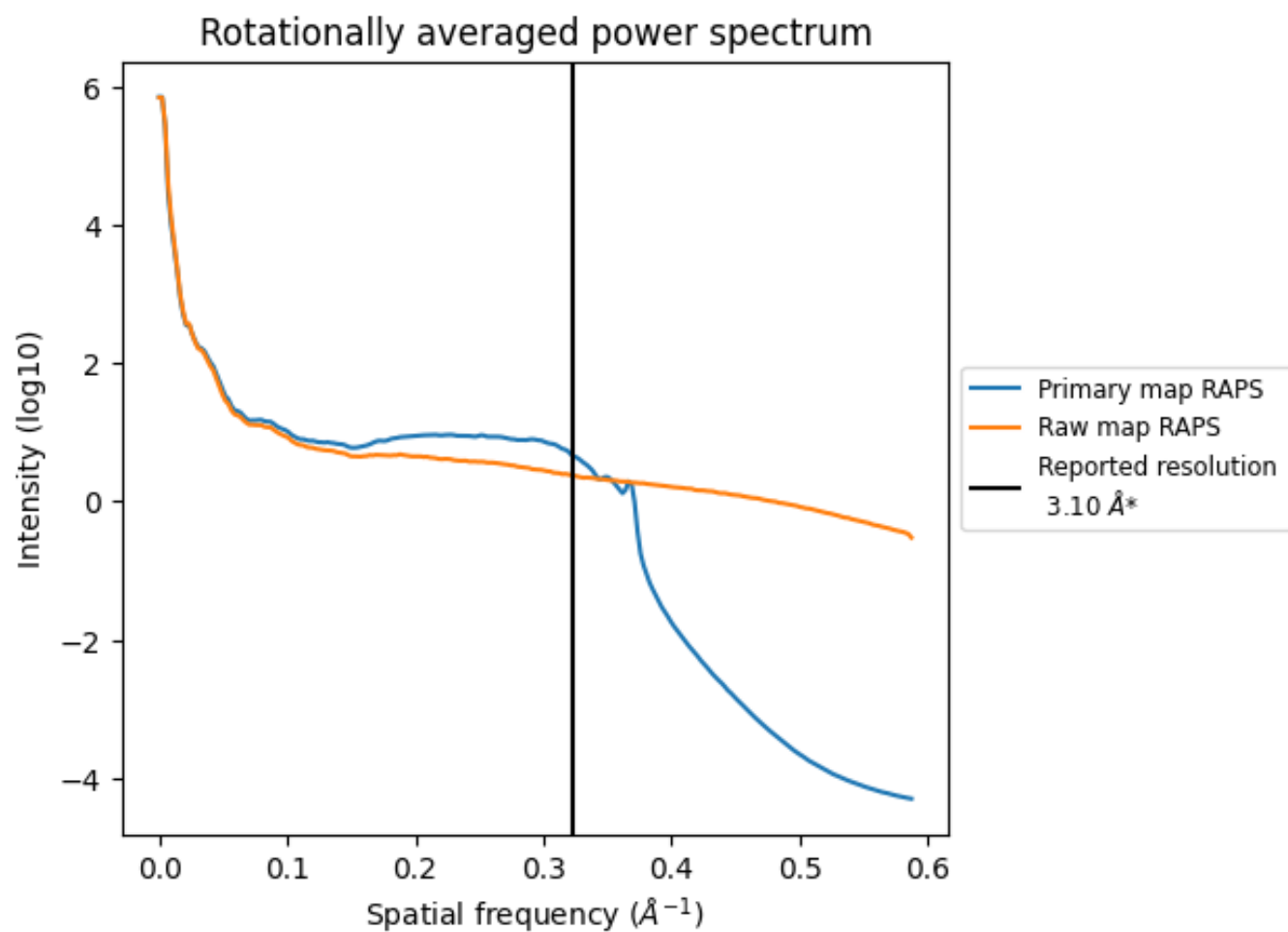
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1601 nm<sup>3</sup>; this corresponds to an approximate mass of 1446 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

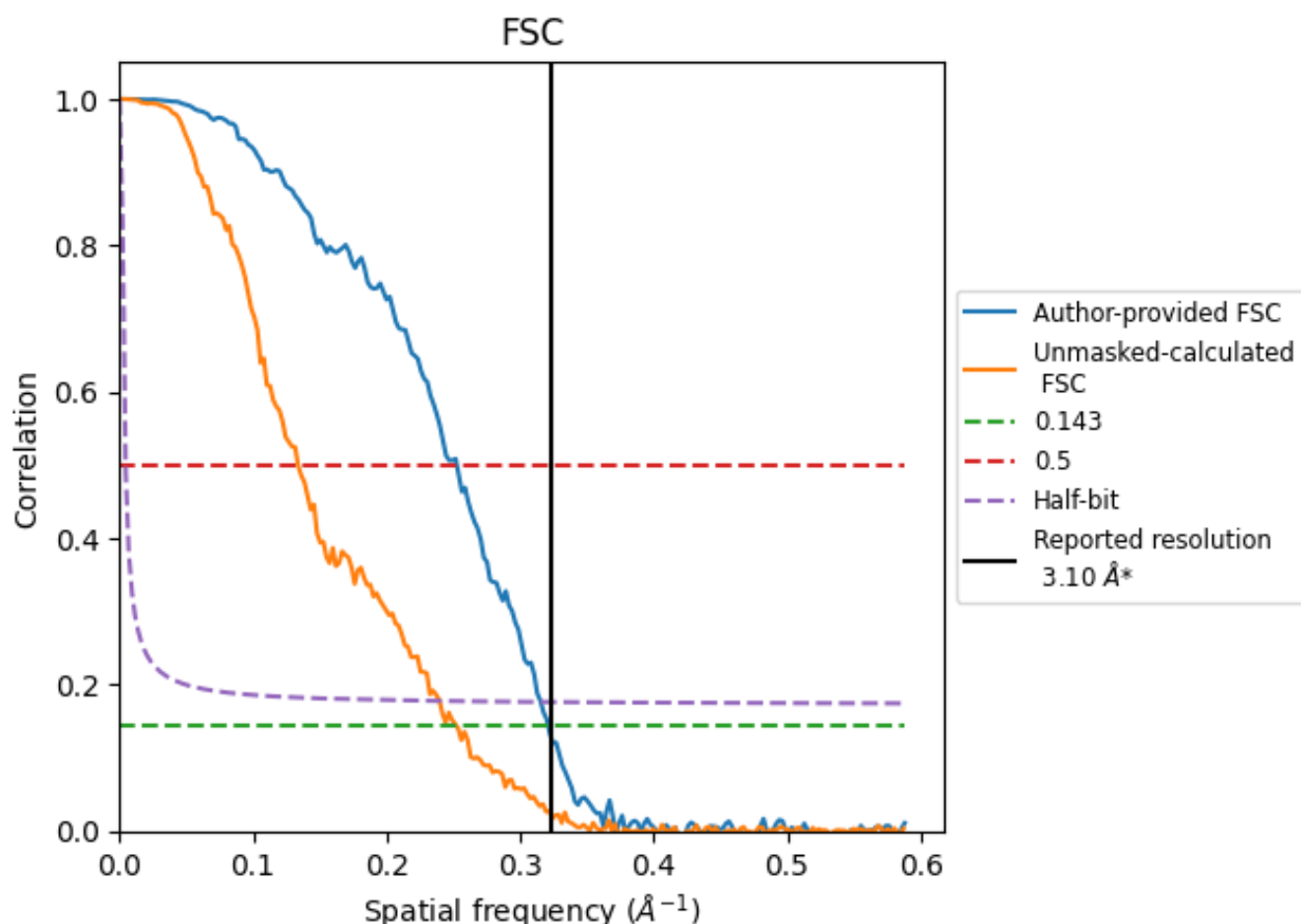


\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

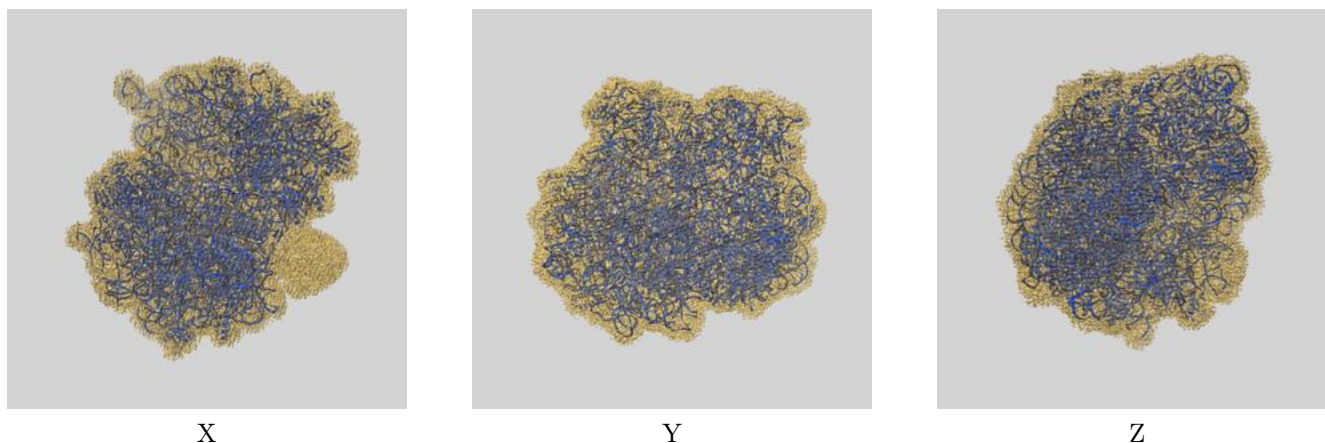
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.96	3.17
Unmasked-calculated*	3.96	7.47	4.17

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

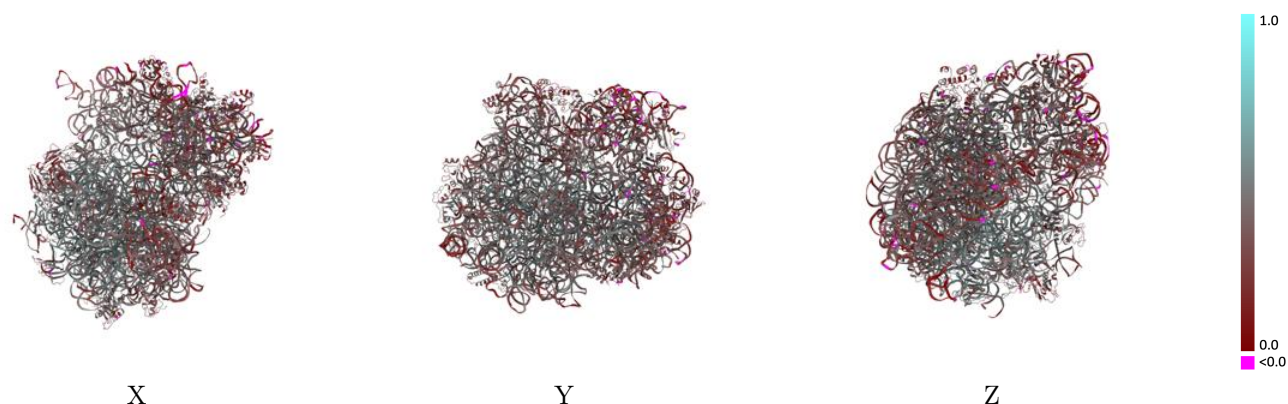
This section contains information regarding the fit between EMDB map EMD-18145 and PDB model 8Q4F. Per-residue inclusion information can be found in section [3](#) on page [14](#).

### 9.1 Map-model overlay [i](#)



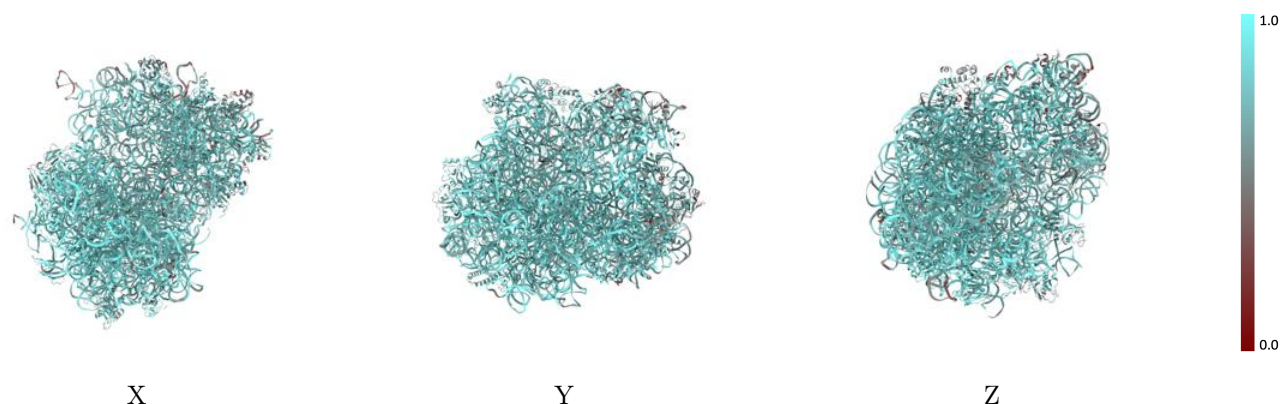
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



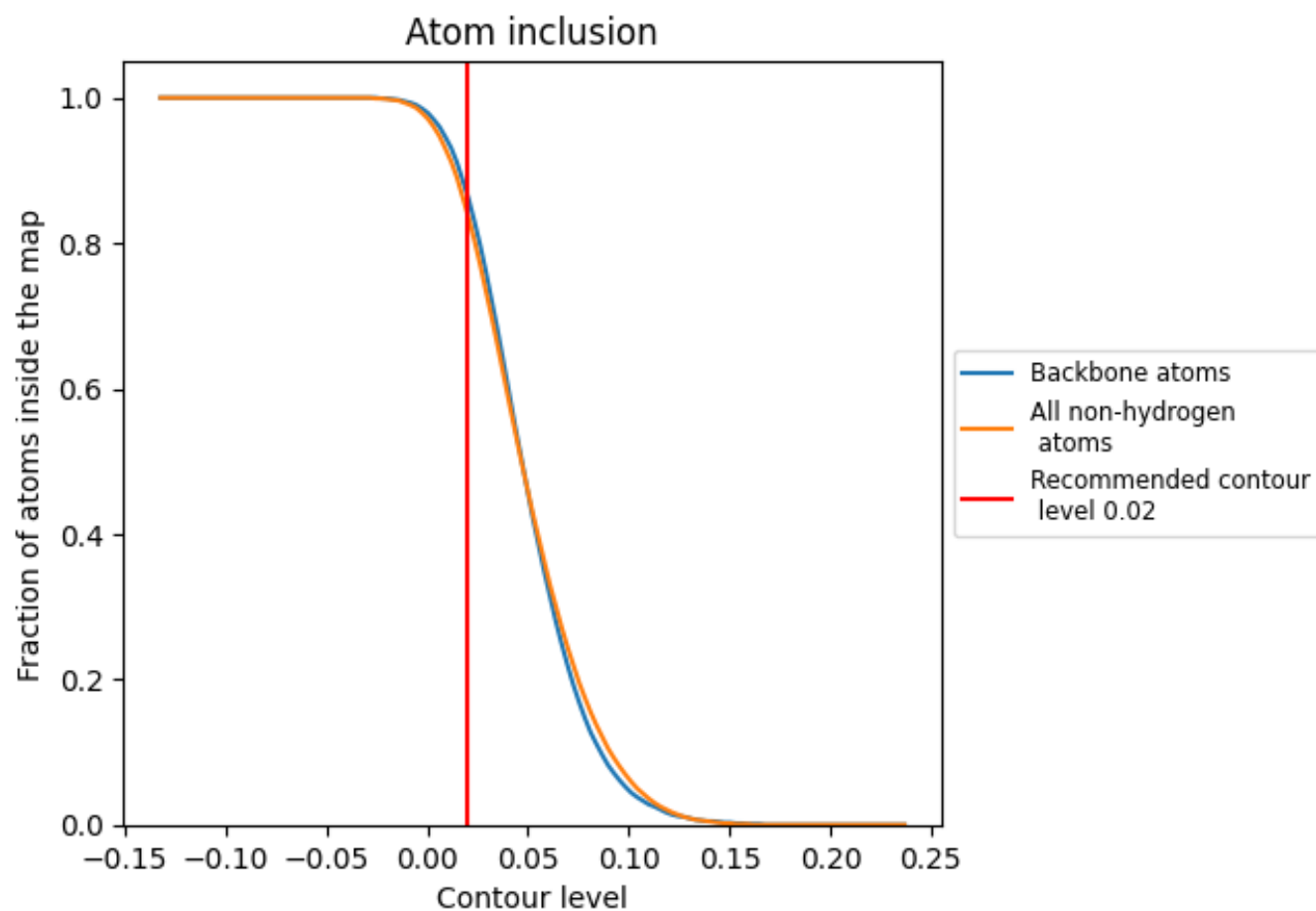
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 87% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ





































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.4010
0	 0.7600	 0.3380
1	 0.8960	 0.4780
2	 0.8110	 0.3820
3	 0.8390	 0.4350
4	 0.6260	 0.2200
A	 0.8310	 0.3660
B	 0.5860	 0.2730
C	 0.7720	 0.3620
D	 0.6630	 0.2830
E	 0.7860	 0.3670
F	 0.7160	 0.3000
G	 0.7120	 0.3130
H	 0.7700	 0.3440
I	 0.7060	 0.3000
J	 0.6460	 0.2790
K	 0.7770	 0.3750
L	 0.7570	 0.3430
M	 0.7100	 0.3110
N	 0.7690	 0.3440
O	 0.8130	 0.3740
P	 0.7500	 0.3120
Q	 0.7490	 0.3330
R	 0.7420	 0.3320
S	 0.7130	 0.3110
T	 0.7370	 0.3280
U	 0.6620	 0.3160
X	 0.9540	 0.5310
Z	 0.8050	 0.3680
a	 0.9000	 0.4510
b	 0.8270	 0.3470
c	 0.8540	 0.4440
d	 0.8670	 0.4710
e	 0.7950	 0.3950
f	 0.7090	 0.3000



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
g	 0.7050	 0.2980
i	 0.8360	 0.4320
j	 0.8500	 0.4380
k	 0.8030	 0.3950
l	 0.8230	 0.4140
m	 0.9050	 0.4910
n	 0.7080	 0.2930
o	 0.8500	 0.4550
p	 0.8330	 0.4240
q	 0.8240	 0.4380
s	 0.8290	 0.4100
t	 0.7950	 0.3900
u	 0.7440	 0.3340
v	 0.7950	 0.3760
w	 0.7890	 0.3680
x	 0.7670	 0.3630
y	 0.8010	 0.3940
z	 0.8390	 0.4420